Batch Systems

Running your jobs on an HPC machine

Reusing this material

Outline

- What is a batch system and why do we need them?
- How do I use a batch system to run my jobs?
  - Concepts
  - Resource scheduling and job execution
  - Job submission scripts
  - Interactive jobs
- Scheduling
- Best practice
- Common batch systems
  - Converting between different batch systems

Batch Systems

What are they and why do we need them?

What is a batch system?

- Mechanism to control access by many users to shared computing resources
- Queuing / scheduling system for users’ jobs
- Manages the reservation of resources and job execution
- Allows users to “fire and forget” large, long calculations or many jobs (“production runs”)

Why do we need a batch system?

- Ensure all users get a fair share of compute resources (demand usually exceeds supply)
- To ensure the machine is utilised as efficiently as possible
- To track usage - for accounting and budget control
- To mediate access to other resources e.g. software licences

Using batch systems

How can I use them to run and manage my jobs?

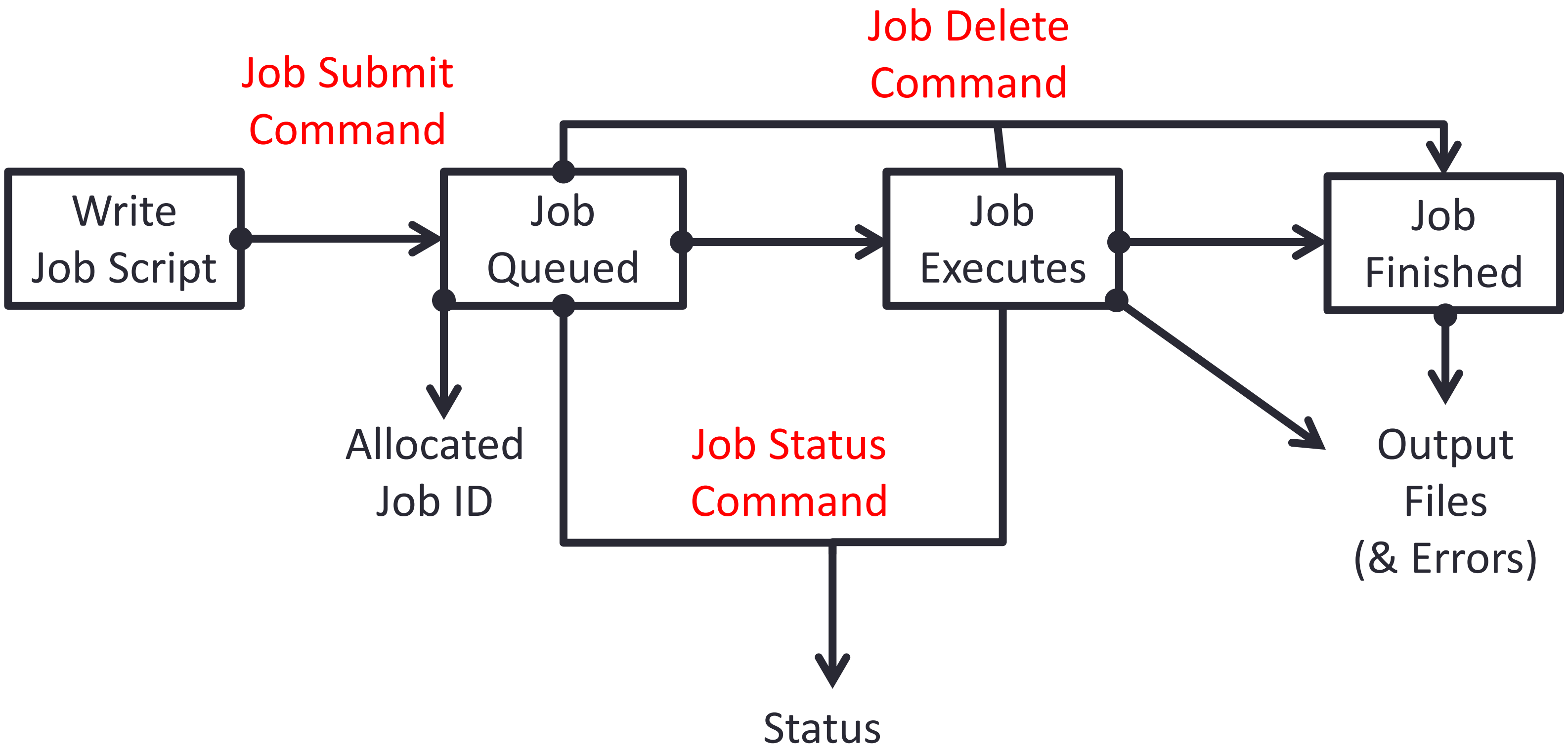
How to use a batch system

1. Set up a job, consisting of:
   - Commands that run one or more calculations / simulations
   - Specification of compute resources needed to do this

2. Submit your job to the batch system
   - Job is placed in a queue by the scheduler
   - Will be executed when there is space and time on the machine
   - Job runs until it finishes successfully, is terminated due to errors, or exceeds a time limit

3. Examine outputs and any error messages

Batch system flow



Resource scheduling & job execution

- When you submit a job to a batch system you specify the resources it requires (number of nodes / cores, job time, etc.)
- The batch system schedules a block of resources that meet these requirements to become available for your job to use
- When it runs your job can use these resources however it likes (specified in advance in your job script):
  - Run a single calculation / simulation that spans all cores and full time
  - Run multiple shorter calculations / simulations in sequence
  - Run multiple smaller calculations / simulations running in parallel for the full time

Batch system concepts

- Queue – a logical scheduling category that may correspond to a portion of the machine:
  - Different time constraints
  - Nodes with special features such as large memory, different processor architecture or accelerators such as GPUs, etc.
  - Nodes reserved for access by a subset of users (e.g. for training)
  - Generally have a small number of defined queues
  - Jobs contend for resources within the queue in which they sit

E.g. on ARCHER:

- "standard" queue (24 hour limit, no limit on number of nodes)
- "short" queue (max 20 minutes & 8 nodes, weekdays 08:00-22:00 only)

Batch system concepts

- Priority – numerical ranking of a job by the scheduler that influences how soon it will start (higher priority more likely to start sooner)

- Account name / budget code – identifier used to charge (£) time used
  - Jobs may be rejected when you submit with insufficient budget

- Walltime – the time a job takes (or is expected to take)

Batch system commands & job states

	PBS (ARCHER & Cirrus)	SLURM
Job submit command	qsub myjob.pbs	sbatch myjob_sbatch
Job status command	qstat –u $USER	squeue –u $USER
Job delete command	qdel #########	scancel #########

PBS job state (ARCHER & Cirrus)	Meaning
Q	The job is *queued* and waiting to start
R	The job is currently *running*
E	The job is currently *exiting*
H	The job is *held* and not eligible to run

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Parallel application launcher commands

Use these commands inside a job script to launch a parallel executable

Parallel application launcher commands	
aprun –n 48 –N 12 –d 2 my_program	(ARCHER)
mpiexec_mpt –n 48 –ppn 24 my_program	(Cirrus)
mpirun –ppn 12 –np 48 my_program	
mpiexec –n 48 my_program	

Job submission scripts

PBS example:

```
#!/bin/bash -login
#PBS -N Weather1
#PBS -l select=200
#PBS -l walltime=1:00:00
#PBS -q short
cd $PBS_O_WORKDIR
aprun -n 4800 weathersim
```

- `#!/bin/bash -login` — Linux shell to run job script in
- `#PBS -N Weather1` — Job name
- `#PBS -l select=200` — Number of nodes requested
- `#PBS -l walltime=1:00:00` — Requested job duration
- `#PBS -q short` — Queue to submit job to
- `cd $PBS_O_WORKDIR` — Changing to directory to run in
- `aprun` — Parallel job launcher
- `-n 4800` — Number of parallel instances of program to launch
- `weathersim` — Program name

Job submission scripts

SLURM example:

```
#!/bin/bash
#SBATCH -J Weather1
#SBATCH --nodes=2
#SBATCH --time=12:00:00
#SBATCH --ntasks=24
#SBATCH -p tesla
mpirun -np 24 weathersim
```

- `#!/bin/bash` — Linux shell to run job script in
- `#SBATCH -J Weather1` — Job name
- `#SBATCH --nodes=2` — Number of nodes requested
- `#SBATCH --time=12:00:00` — Requested job duration
- `#SBATCH --ntasks=24` — Number of parallel tasks
- `#SBATCH -p tesla` — Queue to submit job to (GPU queue)
- `mpirun` — Parallel job launcher
- `-np 24` — Number of parallel instances of program to launch
- `weathersim` — Program name

Interactive jobs

- Most HPC machines allow both batch and interactive jobs

- **Batch jobs** are non-interactive.
  - You write a *job submission script* to run your job
  - Jobs run without user intervention and you collect results at the end
- **Interactive jobs** allow you to use compute resources interactively
  - For testing, debugging/profiling, software development work
  - For visualisation and data analysis
- How these are set up and charged varies from machine to machine

Interactive jobs

- If using the same compute resource as batch jobs then need to request interactive jobs from the batch scheduler
  - Use same resource request variables as batch jobs (duration, size)
  - Wait until job runs to get an interactive session
  - Within interactive session run serial code or parallel programs using parallel launcher as for batch jobs
- May have a small part of the HPC machine dedicated to interactive jobs
  - Typically for visualisation & postprocessing / data analysis
  - May bypass the batch scheduler for instant access
  - May be limited in performance, available libraries, parallelism, etc.

Scheduling of jobs

A brief look under the hood at when jobs are run

Scheduling

- Complex scheduling algorithms try to run many jobs of different sizes on system to ensure maximum utilisation and minimum wait time

- Batch schedulers can implement scheduling policy that varies from machine to machine by allowing control over the relative importance to job prioritisation of:
  - Waiting times
  - Large vs small jobs
  - Long vs short jobs
  - Power consumption

Scheduling

- Backfilling:
  - Assign all jobs priority according to policy & scheduling algorithm
  - Starting with highest priority job, run each lesser priority job that can run with current free resources
  - For the highest priority job *A* that can not currently run, calculate when the required resources will become available and schedule job *A* to run at this time.
  - Until such time, run any less high priority jobs that will complete before job *A* starts and for which sufficient resources are currently available
  - This "fills gaps" and improves resource utilisation

- Active area of research
- For example on ARCHER you can view detailed statistics on this
  - http://archer.ac.uk/status/

- How long until my job executes?
  - Not always an easy question to answer!

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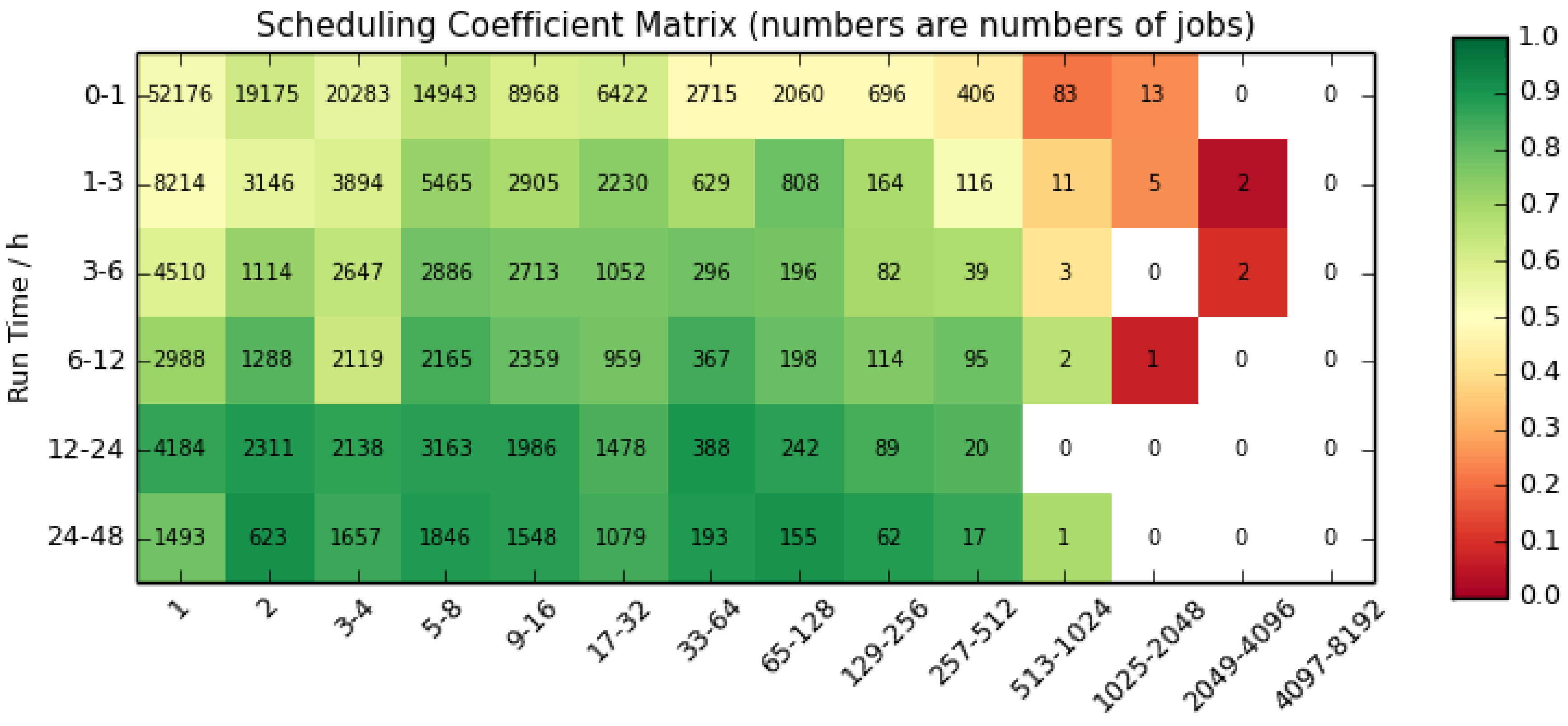
Scheduling


Scheduling Coefficient Matrix (numbers are numbers of jobs)
Run Time / h
0-1
1-3
3-6
6-12
12-24
24-48
52176 19175 20283 14943 8968 6422 2715 2060 696 406 83 13 0 0
8214 3146 3894 5465 2905 2230 629 808 164 116 11 5 2 0
4510 1114 2647 2886 2713 1052 296 196 82 39 3 0 2 0
2988 1288 2119 2165 2359 959 367 198 114 95 2 1 0 0
4184 2311 2138 3163 1986 1478 388 242 89 20 0 0 0 0
1493 623 1657 1846 1548 1079 193 155 62 17 1 0 0 0
1
2
3-4
5-8
9-16
17-32
33-64
65-128
129-256
257-512
513-1024
1025-2048
2049-4096
4097-8192
Job Size / nodes
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0

Best practice

Tips for making the most effective use of batch systems

Best practice

- Run short tests using interactive jobs if possible
- Once you are happy the setup works write a short test job script and submit it to the batch system
- Finally, produce scripts for full production runs

- Remember you have the full functionality of the Linux command line (bash or other) available in scripts
  - This allows for sophisticated scripts if you need them
  - Can automate a lot of tedious data analysis and transformation
  - …be careful to test when moving, copying deleting important data – it is very easy to lose the results of a large simulation due to a typo (or unforeseen error) in a script

Migrating

Changing your scripts from one batch system to another

Batch systems

- PBS (on ARCHER and Cirrus), Torque
- Grid Engine
- SLURM
- LSF – IBM Systems
- LoadLeveller – IBM Systems

- It is not unusual for applications to run over many different HPC machines which might be using different queue systems
  - You often see sets of submission scripts for different systems
  - From a user's perspective different commands are used to submit and manage jobs

Submission script conversion

- Usually need to change the batch system options
- Sometimes need to change the commands in the script
  - Particularly to different paths
  - Usually the order (logic) of the commands remains the same

- Tends to be a fairly mechanical process and there are some utilities that can help
  - Bolt – from EPCC, generates job submission scripts for a variety of batch systems/HPC resources: https://github.com/aturner-epcc/bolt

- HPC machine documentation often provides significant reference material
  - Especially true for ARCHER and Cirrus

Summary

Summary

- Submitting jobs through a batch system represents a different way of interacting with a computer than you might be used to
  - But this has a crucial role in enabling potentially thousands of users to easily run jobs on the same machine concurrently

- A number of different batch system technologies
  - Fundamentally the same concepts, but different options and commands
  - These are all well documented
  - Many applications are shipped with submission scripts for multiple systems